

## metal-organic compounds

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

**cis-Dichloridobis(trimethoxyphosphine)palladium(II) at 125 K****Alexandra M. Z. Slawin, Paul G. Waddell and J. Derek Woollins\***Department of Chemistry, University of St Andrews, St Andrews, KY16 9ST, Scotland  
Correspondence e-mail: [jdw3@st-and.ac.uk](mailto:jdw3@st-and.ac.uk)

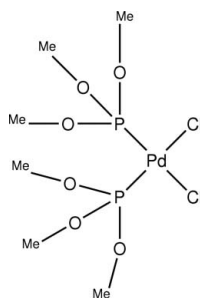
Received 19 August 2009; accepted 13 October 2009

Key indicators: single-crystal X-ray study;  $T = 125$  K; mean  $\sigma(\text{O}-\text{C}) = 0.010$  Å;  $R$  factor = 0.054;  $wR$  factor = 0.090; data-to-parameter ratio = 16.4.

The title compound,  $[\text{PdCl}_2(\text{C}_3\text{H}_9\text{O}_3\text{P})_2]$ , which is isotypic with its platinum analogue, adopts a slightly distorted *cis* square-planar geometry for the Pd centre.

**Related literature**

For the platinum analogue, see: Bao *et al.* (1987). For related platinum complexes, see: Slawin *et al.* (2007*a,b*). For *cis*-bis-(triisopropoxyphosphino)platinum dichloride, see: Slawin *et al.* (2009).

**Experimental***Crystal data* $[\text{PdCl}_2(\text{C}_3\text{H}_9\text{O}_3\text{P})_2]$  $M_r = 425.46$ Monoclinic, *Cc* $a = 6.8059$  (19) Å $b = 16.897$  (5) Å $c = 13.374$  (4) Å $\beta = 100.086$  (7)° $V = 1514.2$  (7) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 1.80$  mm<sup>-1</sup> $T = 125$  K $0.22 \times 0.16 \times 0.13$  mm*Data collection*

Rigaku SCXmini diffractometer

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

 $T_{\min} = 0.662$ ,  $T_{\max} = 0.791$ 

6333 measured reflections

2639 independent reflections

2338 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.072$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.054$  $wR(F^2) = 0.090$  $S = 1.07$ 

2639 reflections

161 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.26$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.71$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

1308 Friedel pairs

Flack parameter:  $-0.01$  (5)**Table 1**

Selected geometric parameters (Å, °).

Pd1—Cl1	2.356 (2)	Pd1—P1	2.241 (2)
Pd1—Cl2	2.358 (2)	Pd1—P2	2.233 (2)
Cl1—Pd1—Cl2	89.71 (8)	Cl2—Pd1—P1	90.32 (8)
Cl1—Pd1—P1	179.04 (9)	Cl2—Pd1—P2	177.30 (8)
Cl1—Pd1—P2	87.59 (8)	P1—Pd1—P2	92.38 (8)

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2006); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FI2085).

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**supplementary materials**

*Acta Cryst.* (2009). E65, m1391 [ doi:10.1107/S1600536809041919 ]

## ***cis*-Dichloridobis(trimethoxyphosphine)palladium(II) at 125 K**

**A. M. Z. Slawin, P. G. Waddell and J. D. Woollins**

### **Comment**

[PdCl<sub>2</sub>(P(OMe)<sub>3</sub>)<sub>2</sub>] is isomorphous with its platinum analogue [PtCl<sub>2</sub>(P(OMe)<sub>3</sub>)<sub>2</sub>] (**2**) (Bao *et al.*, 1987) and adopts a *cis* square planar geometry. Whereas the Pt complex was reported to have quite dissimilar bond lengths for Pt—P1/Pt—P2 and Pt—Cl1/PtCl2 bond lengths these pairs of bonds are equivalent in the title compound.

The Pd—Cl bond bonds in (**1**) ( Pd(1)—Cl(1) 2.356?(2), Pd(1)—Cl(2) 2.358?(2) Å ) are shorter than the Pt—Cl bonds in (**2**) whilst the Pd—P bonds ( Pd(1)—P(1) 2.241?(2), Pd(1)—P(2) 2.233?(2) Å ) are longer than the Pt—P bonds in (**2**). The P—M—P angle ( P(1)—Pd(1)—P(2) 92.38?(8) ° ) is reduced and the Cl—M—Cl angle is enlarged ( Cl(1)—Pd(1)—Cl(2) 89.71?(8) ° ) on going from Pt to Pd with the palladium compound reported here having angles which are closer to ideal square planar .

### **Experimental**

0.5 g (1.75 mmol) of PdCl<sub>2</sub>(COD) was dissolved in dichloromethane (5 mL) in a round-bottomed flask. To this 0.41 mL (3.5 mmol) of trimethylphosphite was added. The solution was stirred for 0.5 h at room temperature. The product was precipitated *via* slow diffusion of hexane and was then filtered off and dried under vacuum, [PdCl<sub>2</sub>(P(OMe)<sub>3</sub>)<sub>2</sub>] (1.36 mmol, *ca* 77%). <sup>31</sup>P-{<sup>1</sup>H}NMR: δ 97.9 p.p.m..

### **Refinement**

All H atoms were included in calculated positions and refined as riding atoms with U<sub>iso</sub>(H) = 1.5 U<sub>eq</sub>. The highest peak in the difference map is 1.097 Å from atom Pd1.

### **Figures**

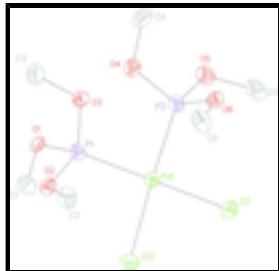


Fig. 1. The structure of the title compound with displacement ellipsoids drawn at the 50% probability level, hydrogen atoms omitted for clarity.

## *cis*-Dichloridobis(trimethoxyphosphine)palladium(II)

### Crystal data

$[\text{PdCl}_2(\text{C}_3\text{H}_9\text{O}_3\text{P})_2]$	$F_{000} = 848.00$
$M_r = 425.46$	$D_x = 1.866 \text{ Mg m}^{-3}$
Monoclinic, <i>Cc</i>	Mo $K\alpha$ radiation, $\lambda = 0.71075 \text{ \AA}$
Hall symbol: C -2yc	Cell parameters from 7139 reflections
$a = 6.8059 (19) \text{ \AA}$	$\theta = 3.1\text{--}27.7^\circ$
$b = 16.897 (5) \text{ \AA}$	$\mu = 1.80 \text{ mm}^{-1}$
$c = 13.374 (4) \text{ \AA}$	$T = 125 \text{ K}$
$\beta = 100.086 (7)^\circ$	Chunk, yellow
$V = 1514.2 (7) \text{ \AA}^3$	$0.22 \times 0.16 \times 0.13 \text{ mm}$
$Z = 4$	

### Data collection

Rigaku SCXmini diffractometer	2639 independent reflections
Radiation source: fine-focus sealed tube	2338 reflections with $F^2 > 2.0\sigma(F^2)$
Monochromator: graphite	$R_{\text{int}} = 0.072$
Detector resolution: $6.85 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 25.4^\circ$
$T = 125 \text{ K}$	$\theta_{\text{min}} = 2.1^\circ$
$\omega$ scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$k = -20 \rightarrow 20$
$T_{\text{min}} = 0.662$ , $T_{\text{max}} = 0.791$	$l = -16 \rightarrow 16$
6333 measured reflections	

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2]$
$wR(F^2) = 0.090$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2639 reflections	$\Delta\rho_{\text{max}} = 1.26 \text{ e \AA}^{-3}$
161 parameters	$\Delta\rho_{\text{min}} = -0.71 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Hydrogen site location: inferred from neighbouring sites	Absolute structure: Flack,(1983), 1308 Friedel pairs
	Flack parameter: $-0.01 (5)$

### Special details

**Geometry.** ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

**Refinement.** Refinement was performed using all reflections. The weighted  $R$ -factor ( $wR$ ) and goodness of fit ( $S$ ) are based on  $F^2$ .  $R$ -factor (gt) are based on  $F$ . The threshold expression of  $F^2 > 2.0 \sigma(F^2)$  is used only for calculating  $R$ -factor (gt).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Pd(1)	0.50973 (10)	0.10743 (4)	0.45788 (7)	0.01777 (16)
Cl(1)	0.4602 (3)	0.23766 (14)	0.39555 (17)	0.0298 (6)
Cl(2)	0.2407 (3)	0.06430 (14)	0.33413 (17)	0.0277 (6)
P(1)	0.5605 (3)	−0.01677 (14)	0.51540 (16)	0.0183 (5)
P(2)	0.7614 (3)	0.15409 (14)	0.57243 (17)	0.0201 (5)
O(1)	0.7314 (8)	−0.0612 (3)	0.4734 (4)	0.0215 (14)
O(2)	0.3841 (8)	−0.0766 (3)	0.4858 (4)	0.0210 (14)
O(3)	0.6237 (9)	−0.0227 (3)	0.6348 (4)	0.0252 (15)
O(4)	0.9294 (8)	0.0917 (3)	0.6089 (4)	0.0259 (15)
O(5)	0.6928 (8)	0.1816 (3)	0.6740 (4)	0.0267 (15)
O(6)	0.8710 (8)	0.2305 (3)	0.5430 (4)	0.0202 (14)
C(1)	0.7285 (16)	−0.0650 (6)	0.3643 (6)	0.034 (2)
C(2)	0.1966 (14)	−0.0676 (5)	0.5230 (7)	0.030 (2)
C(3)	0.6711 (15)	−0.0993 (5)	0.6843 (7)	0.033 (2)
C(4)	1.1106 (14)	0.1149 (5)	0.6777 (7)	0.036 (2)
C(5)	0.5731 (15)	0.2526 (5)	0.6788 (6)	0.032 (2)
C(6)	0.9618 (13)	0.2290 (5)	0.4527 (8)	0.032 (2)
H(1)	0.7662	−0.1183	0.3459	0.041*
H(2)	0.8233	−0.0265	0.3455	0.041*
H(3)	0.5939	−0.0527	0.3281	0.041*
H(4)	0.2211	−0.0723	0.5972	0.037*
H(5)	0.1031	−0.1090	0.4935	0.037*
H(6)	0.1394	−0.0155	0.5034	0.037*
H(7)	0.6000	−0.1045	0.7417	0.040*
H(8)	0.8152	−0.1028	0.7089	0.040*
H(9)	0.6298	−0.1419	0.6354	0.040*
H(10)	1.2047	0.1387	0.6388	0.043*
H(11)	1.1716	0.0681	0.7138	0.043*
H(12)	1.0774	0.1534	0.7269	0.043*
H(13)	0.6614	0.2980	0.6975	0.038*
H(14)	0.4874	0.2454	0.7298	0.038*
H(15)	0.4901	0.2621	0.6123	0.038*
H(16)	1.0930	0.2546	0.4672	0.038*
H(17)	0.8764	0.2575	0.3977	0.038*
H(18)	0.9775	0.1740	0.4321	0.038*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Pd(1)	0.0217 (3)	0.0152 (3)	0.0159 (3)	0.0006 (3)	0.0018 (2)	−0.0001 (3)
Cl(1)	0.0375 (15)	0.0183 (13)	0.0301 (14)	0.0010 (12)	−0.0040 (11)	0.0048 (10)
Cl(2)	0.0321 (14)	0.0253 (14)	0.0223 (13)	−0.0027 (12)	−0.0050 (11)	0.0006 (10)

## supplementary materials

P(1)	0.0228 (14)	0.0171 (13)	0.0157 (13)	−0.0017 (11)	0.0056 (10)	−0.0012 (9)
P(2)	0.0234 (15)	0.0173 (14)	0.0193 (13)	−0.0010 (11)	0.0031 (11)	−0.0002 (10)
O(1)	0.031 (3)	0.019 (3)	0.014 (3)	0.013 (3)	0.003 (2)	0.002 (2)
O(2)	0.024 (3)	0.019 (3)	0.020 (3)	0.001 (2)	0.004 (2)	0.004 (2)
O(3)	0.038 (4)	0.019 (3)	0.016 (3)	0.005 (3)	−0.002 (2)	0.002 (2)
O(4)	0.021 (3)	0.017 (3)	0.037 (3)	0.000 (2)	−0.003 (3)	−0.001 (2)
O(5)	0.036 (4)	0.026 (3)	0.019 (3)	0.000 (3)	0.006 (2)	−0.002 (2)
O(6)	0.025 (3)	0.019 (3)	0.017 (3)	0.000 (2)	0.005 (2)	0.004 (2)
C(1)	0.050 (7)	0.038 (6)	0.014 (5)	0.015 (5)	0.006 (5)	−0.010 (4)
C(2)	0.030 (6)	0.026 (5)	0.036 (6)	−0.002 (5)	0.008 (4)	−0.002 (5)
C(3)	0.046 (6)	0.024 (5)	0.030 (5)	0.006 (5)	0.006 (4)	−0.002 (4)
C(4)	0.026 (5)	0.029 (6)	0.047 (6)	0.006 (4)	−0.007 (4)	0.007 (5)
C(5)	0.045 (6)	0.036 (6)	0.016 (5)	−0.003 (5)	0.011 (4)	−0.009 (4)
C(6)	0.037 (8)	0.028 (5)	0.033 (5)	−0.005 (4)	0.013 (5)	−0.008 (5)

### *Geometric parameters (Å, °)*

Pd(1)—Cl(1)	2.356 (2)	C(1)—H(2)	0.980
Pd(1)—Cl(2)	2.358 (2)	C(1)—H(3)	0.980
Pd(1)—P(1)	2.241 (2)	C(2)—H(4)	0.980
Pd(1)—P(2)	2.233 (2)	C(2)—H(5)	0.980
P(1)—O(1)	1.568 (6)	C(2)—H(6)	0.980
P(1)—O(2)	1.567 (6)	C(3)—H(7)	0.980
P(1)—O(3)	1.583 (5)	C(3)—H(8)	0.980
P(2)—O(4)	1.568 (6)	C(3)—H(9)	0.980
P(2)—O(5)	1.582 (6)	C(4)—H(10)	0.980
P(2)—O(6)	1.575 (6)	C(4)—H(11)	0.980
O(1)—C(1)	1.457 (10)	C(4)—H(12)	0.980
O(2)—C(2)	1.457 (12)	C(5)—H(13)	0.980
O(3)—C(3)	1.464 (10)	C(5)—H(14)	0.980
O(4)—C(4)	1.458 (10)	C(5)—H(15)	0.980
O(5)—C(5)	1.458 (11)	C(6)—H(16)	0.980
O(6)—C(6)	1.451 (12)	C(6)—H(17)	0.980
C(1)—H(1)	0.980	C(6)—H(18)	0.980
Cl(1)···O(5) <sup>i</sup>	3.473 (5)	H(4)···O(6) <sup>iii</sup>	3.594
Cl(1)···C(5) <sup>i</sup>	3.563 (8)	H(4)···C(4) <sup>viii</sup>	3.466
O(1)···C(2) <sup>ii</sup>	3.121 (11)	H(4)···C(5) <sup>iii</sup>	3.367
O(2)···O(6) <sup>iii</sup>	3.352 (7)	H(4)···H(8) <sup>viii</sup>	3.402
O(2)···C(6) <sup>iii</sup>	3.367 (10)	H(4)···H(11) <sup>viii</sup>	2.891
O(3)···C(1) <sup>iv</sup>	3.369 (10)	H(4)···H(13) <sup>iii</sup>	2.636
O(4)···C(2) <sup>ii</sup>	3.550 (11)	H(4)···H(15) <sup>iii</sup>	3.232
O(5)···Cl(1) <sup>v</sup>	3.473 (5)	H(5)···Cl(1) <sup>iii</sup>	2.989
O(5)···C(1) <sup>iv</sup>	3.194 (11)	H(5)···O(1) <sup>viii</sup>	2.624
O(6)···O(2) <sup>vi</sup>	3.352 (7)	H(5)···O(6) <sup>iii</sup>	3.271
C(1)···O(3) <sup>vii</sup>	3.369 (10)	H(5)···C(1) <sup>viii</sup>	2.915
C(1)···O(5) <sup>vii</sup>	3.194 (11)	H(5)···C(5) <sup>iii</sup>	3.440

C(1)···C(2) <sup>ii</sup>	3.506 (13)	H(5)···H(1) <sup>viii</sup>	2.756
C(2)···O(1) <sup>viii</sup>	3.121 (11)	H(5)···H(2) <sup>viii</sup>	2.858
C(2)···O(4) <sup>viii</sup>	3.550 (11)	H(5)···H(13) <sup>iii</sup>	3.113
C(2)···C(1) <sup>viii</sup>	3.506 (13)	H(5)···H(15) <sup>iii</sup>	2.879
C(5)···Cl(1) <sup>v</sup>	3.563 (8)	H(5)···H(17) <sup>iii</sup>	3.321
C(6)···O(2) <sup>vi</sup>	3.367 (10)	H(6)···O(1) <sup>viii</sup>	2.842
Pd(1)···H(7) <sup>vii</sup>	3.060	H(6)···O(4) <sup>viii</sup>	2.832
Pd(1)···H(10) <sup>viii</sup>	3.493	H(6)···C(1) <sup>viii</sup>	3.188
Cl(1)···H(1) <sup>ix</sup>	2.793	H(6)···C(4) <sup>viii</sup>	3.238
Cl(1)···H(5) <sup>vi</sup>	2.989	H(6)···H(1) <sup>viii</sup>	3.469
Cl(1)···H(7) <sup>vii</sup>	3.300	H(6)···H(2) <sup>viii</sup>	2.745
Cl(1)···H(12) <sup>i</sup>	3.121	H(6)···H(10) <sup>viii</sup>	3.158
Cl(1)···H(13) <sup>i</sup>	3.103	H(6)···H(11) <sup>viii</sup>	3.121
Cl(1)···H(14) <sup>i</sup>	3.585	H(6)···H(18) <sup>viii</sup>	3.466
Cl(1)···H(16) <sup>viii</sup>	2.843	H(7)···Pd(1) <sup>iv</sup>	3.060
Cl(1)···H(18) <sup>viii</sup>	3.571	H(7)···Cl(1) <sup>iv</sup>	3.300
Cl(2)···H(2) <sup>viii</sup>	3.255	H(7)···Cl(2) <sup>iv</sup>	3.005
Cl(2)···H(4) <sup>vii</sup>	3.151	H(7)···C(1) <sup>iv</sup>	3.339
Cl(2)···H(7) <sup>vii</sup>	3.005	H(7)···H(2) <sup>iv</sup>	2.897
Cl(2)···H(8) <sup>x</sup>	3.149	H(7)···H(3) <sup>iv</sup>	2.900
Cl(2)···H(11) <sup>x</sup>	2.747	H(7)···H(13) <sup>iii</sup>	3.370
Cl(2)···H(13) <sup>i</sup>	2.949	H(7)···H(18) <sup>iv</sup>	3.489
Cl(2)···H(18) <sup>viii</sup>	3.031	H(8)···Cl(2) <sup>xiv</sup>	3.149
O(1)···H(4) <sup>ii</sup>	3.457	H(8)···C(5) <sup>xi</sup>	3.076
O(1)···H(5) <sup>ii</sup>	2.624	H(8)···H(2) <sup>iv</sup>	2.842
O(1)···H(6) <sup>ii</sup>	2.842	H(8)···H(3) <sup>iv</sup>	3.543
O(1)···H(16) <sup>iii</sup>	3.250	H(8)···H(4) <sup>ii</sup>	3.402
O(2)···H(16) <sup>iii</sup>	3.216	H(8)···H(13) <sup>xi</sup>	2.917
O(2)···H(17) <sup>iii</sup>	3.038	H(8)···H(14) <sup>xi</sup>	2.814
O(3)···H(2) <sup>iv</sup>	3.022	H(8)···H(15) <sup>xi</sup>	2.973
O(3)···H(3) <sup>iv</sup>	2.920	H(8)···H(18) <sup>iv</sup>	3.229
O(4)···H(1) <sup>iv</sup>	3.567	H(9)···O(6) <sup>iii</sup>	2.917
O(4)···H(2) <sup>iv</sup>	3.543	H(9)···C(5) <sup>xi</sup>	3.465
O(4)···H(4) <sup>ii</sup>	3.429	H(9)···C(6) <sup>iii</sup>	3.325
O(4)···H(6) <sup>ii</sup>	2.832	H(9)···H(13) <sup>iii</sup>	3.578
O(5)···H(1) <sup>iv</sup>	2.506	H(9)···H(14) <sup>xi</sup>	3.173
O(5)···H(2) <sup>iv</sup>	3.494	H(9)···H(15) <sup>xi</sup>	3.001
O(5)···H(3) <sup>iv</sup>	3.151	H(9)···H(16) <sup>iii</sup>	2.826
O(5)···H(10) <sup>viii</sup>	3.352	H(10)···Pd(1) <sup>ii</sup>	3.493
O(6)···H(4) <sup>vi</sup>	3.594	H(10)···O(5) <sup>ii</sup>	3.352
O(6)···H(5) <sup>vi</sup>	3.271	H(10)···C(5) <sup>ii</sup>	3.132

## supplementary materials

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O(6)···H(9) <sup>vi</sup>	2.917	H(10)···H(6) <sup>ii</sup>	3.158
C(1)···H(5) <sup>ii</sup>	2.915	H(10)···H(14) <sup>ii</sup>	2.759
C(1)···H(6) <sup>ii</sup>	3.188	H(10)···H(15) <sup>ii</sup>	2.914
C(1)···H(7) <sup>vii</sup>	3.339	H(11)···Cl(2) <sup>xiv</sup>	2.747
C(1)···H(12) <sup>vii</sup>	3.575	H(11)···C(2) <sup>ii</sup>	3.457
C(1)···H(16) <sup>iii</sup>	3.534	H(11)···H(2) <sup>iv</sup>	3.268
C(2)···H(1) <sup>viii</sup>	3.535	H(11)···H(3) <sup>xiv</sup>	3.021
C(2)···H(2) <sup>viii</sup>	3.235	H(11)···H(4) <sup>ii</sup>	2.891
C(2)···H(11) <sup>viii</sup>	3.457	H(11)···H(6) <sup>ii</sup>	3.121
C(2)···H(13) <sup>iii</sup>	3.293	H(12)···Cl(1) <sup>v</sup>	3.121
C(2)···H(15) <sup>iii</sup>	3.502	H(12)···C(1) <sup>iv</sup>	3.575
C(3)···H(2) <sup>iv</sup>	3.075	H(12)···H(1) <sup>iv</sup>	2.925
C(3)···H(3) <sup>iv</sup>	3.305	H(12)···H(2) <sup>iv</sup>	3.327
C(3)···H(14) <sup>xi</sup>	3.381	H(12)···H(14) <sup>ii</sup>	3.188
C(3)···H(15) <sup>xi</sup>	3.443	H(12)···H(17) <sup>v</sup>	3.161
C(4)···H(1) <sup>iv</sup>	3.522	H(13)···Cl(1) <sup>v</sup>	3.103
C(4)···H(2) <sup>iv</sup>	3.554	H(13)···Cl(2) <sup>v</sup>	2.949
C(4)···H(4) <sup>ii</sup>	3.466	H(13)···C(2) <sup>vi</sup>	3.293
C(4)···H(6) <sup>ii</sup>	3.238	H(13)···H(4) <sup>vi</sup>	2.636
C(4)···H(14) <sup>ii</sup>	3.361	H(13)···H(5) <sup>vi</sup>	3.113
C(5)···H(1) <sup>iv</sup>	3.293	H(13)···H(7) <sup>vi</sup>	3.370
C(5)···H(4) <sup>vi</sup>	3.367	H(13)···H(8) <sup>ix</sup>	2.917
C(5)···H(5) <sup>vi</sup>	3.440	H(13)···H(9) <sup>vi</sup>	3.578
C(5)···H(8) <sup>ix</sup>	3.076	H(14)···Cl(1) <sup>v</sup>	3.585
C(5)···H(9) <sup>ix</sup>	3.465	H(14)···C(3) <sup>ix</sup>	3.381
C(5)···H(10) <sup>viii</sup>	3.132	H(14)···C(4) <sup>viii</sup>	3.361
C(5)···H(17) <sup>xii</sup>	3.430	H(14)···C(6) <sup>xii</sup>	3.047
C(6)···H(9) <sup>vi</sup>	3.325	H(14)···H(1) <sup>iv</sup>	3.097
C(6)···H(14) <sup>xiii</sup>	3.047	H(14)···H(3) <sup>iv</sup>	3.538
H(1)···Cl(1) <sup>xi</sup>	2.793	H(14)···H(8) <sup>ix</sup>	2.814
H(1)···O(4) <sup>vii</sup>	3.567	H(14)···H(9) <sup>ix</sup>	3.173
H(1)···O(5) <sup>vii</sup>	2.506	H(14)···H(10) <sup>viii</sup>	2.759
H(1)···C(2) <sup>ii</sup>	3.535	H(14)···H(12) <sup>viii</sup>	3.188
H(1)···C(4) <sup>vii</sup>	3.522	H(14)···H(16) <sup>xii</sup>	3.131
H(1)···C(5) <sup>vii</sup>	3.293	H(14)···H(17) <sup>xii</sup>	2.492
H(1)···H(5) <sup>ii</sup>	2.756	H(14)···H(18) <sup>xii</sup>	3.040
H(1)···H(6) <sup>ii</sup>	3.469	H(15)···C(2) <sup>vi</sup>	3.502
H(1)···H(12) <sup>vii</sup>	2.925	H(15)···C(3) <sup>ix</sup>	3.443
H(1)···H(14) <sup>vii</sup>	3.097	H(15)···H(4) <sup>vi</sup>	3.232
H(1)···H(16) <sup>iii</sup>	3.050	H(15)···H(5) <sup>vi</sup>	2.879
H(1)···H(17) <sup>iii</sup>	3.545	H(15)···H(8) <sup>ix</sup>	2.973



H(2)···Cl(2) <sup>ii</sup>	3.255	H(15)···H(9) <sup>ix</sup>	3.001
H(2)···O(3) <sup>vii</sup>	3.022	H(15)···H(10) <sup>viii</sup>	2.914
H(2)···O(4) <sup>vii</sup>	3.543	H(15)···H(16) <sup>viii</sup>	3.041
H(2)···O(5) <sup>vii</sup>	3.494	H(16)···Cl(1) <sup>ii</sup>	2.843
H(2)···C(2) <sup>ii</sup>	3.235	H(16)···O(1) <sup>vi</sup>	3.250
H(2)···C(3) <sup>vii</sup>	3.075	H(16)···O(2) <sup>vi</sup>	3.216
H(2)···C(4) <sup>vii</sup>	3.554	H(16)···C(1) <sup>vi</sup>	3.534
H(2)···H(5) <sup>ii</sup>	2.858	H(16)···H(1) <sup>vi</sup>	3.050
H(2)···H(6) <sup>ii</sup>	2.745	H(16)···H(9) <sup>vi</sup>	2.826
H(2)···H(7) <sup>vii</sup>	2.897	H(16)···H(14) <sup>xiii</sup>	3.131
H(2)···H(8) <sup>vii</sup>	2.842	H(16)···H(15) <sup>ii</sup>	3.041
H(2)···H(11) <sup>vii</sup>	3.268	H(17)···O(2) <sup>vi</sup>	3.038
H(2)···H(12) <sup>vii</sup>	3.327	H(17)···C(5) <sup>xiii</sup>	3.430
H(3)···O(3) <sup>vii</sup>	2.920	H(17)···H(1) <sup>vi</sup>	3.545
H(3)···O(5) <sup>vii</sup>	3.151	H(17)···H(5) <sup>vi</sup>	3.321
H(3)···C(3) <sup>vii</sup>	3.305	H(17)···H(12) <sup>i</sup>	3.161
H(3)···H(7) <sup>vii</sup>	2.900	H(17)···H(14) <sup>xiii</sup>	2.492
H(3)···H(8) <sup>vii</sup>	3.543	H(18)···Cl(1) <sup>ii</sup>	3.571
H(3)···H(11) <sup>x</sup>	3.021	H(18)···Cl(2) <sup>ii</sup>	3.031
H(3)···H(14) <sup>vii</sup>	3.538	H(18)···H(6) <sup>ii</sup>	3.466
H(4)···Cl(2) <sup>iv</sup>	3.151	H(18)···H(7) <sup>vii</sup>	3.489
H(4)···O(1) <sup>viii</sup>	3.457	H(18)···H(8) <sup>vii</sup>	3.229
H(4)···O(4) <sup>viii</sup>	3.429	H(18)···H(14) <sup>xiii</sup>	3.040
Cl(1)—Pd(1)—Cl(2)	89.71 (8)	O(2)—C(2)—H(4)	109.5
Cl(1)—Pd(1)—P(1)	179.04 (9)	O(2)—C(2)—H(5)	109.5
Cl(1)—Pd(1)—P(2)	87.59 (8)	O(2)—C(2)—H(6)	109.5
Cl(2)—Pd(1)—P(1)	90.32 (8)	H(4)—C(2)—H(5)	109.5
Cl(2)—Pd(1)—P(2)	177.30 (8)	H(4)—C(2)—H(6)	109.5
P(1)—Pd(1)—P(2)	92.38 (8)	H(5)—C(2)—H(6)	109.5
Pd(1)—P(1)—O(1)	113.9 (2)	O(3)—C(3)—H(7)	109.5
Pd(1)—P(1)—O(2)	116.9 (2)	O(3)—C(3)—H(8)	109.5
Pd(1)—P(1)—O(3)	113.8 (2)	O(3)—C(3)—H(9)	109.5
O(1)—P(1)—O(2)	100.6 (3)	H(7)—C(3)—H(8)	109.5
O(1)—P(1)—O(3)	104.1 (3)	H(7)—C(3)—H(9)	109.5
O(2)—P(1)—O(3)	106.0 (3)	H(8)—C(3)—H(9)	109.5
Pd(1)—P(2)—O(4)	113.9 (2)	O(4)—C(4)—H(10)	109.5
Pd(1)—P(2)—O(5)	112.8 (2)	O(4)—C(4)—H(11)	109.5
Pd(1)—P(2)—O(6)	117.3 (2)	O(4)—C(4)—H(12)	109.5
O(4)—P(2)—O(5)	103.9 (3)	H(10)—C(4)—H(11)	109.5
O(4)—P(2)—O(6)	106.1 (3)	H(10)—C(4)—H(12)	109.5
O(5)—P(2)—O(6)	101.4 (3)	H(11)—C(4)—H(12)	109.5
P(1)—O(1)—C(1)	119.9 (5)	O(5)—C(5)—H(13)	109.5
P(1)—O(2)—C(2)	121.6 (5)	O(5)—C(5)—H(14)	109.5
P(1)—O(3)—C(3)	120.7 (5)	O(5)—C(5)—H(15)	109.5

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P(2)—O(4)—C(4)	120.4 (5)	H(13)—C(5)—H(14)	109.5
P(2)—O(5)—C(5)	122.1 (5)	H(13)—C(5)—H(15)	109.5
P(2)—O(6)—C(6)	118.9 (5)	H(14)—C(5)—H(15)	109.5
O(1)—C(1)—H(1)	109.5	O(6)—C(6)—H(16)	109.5
O(1)—C(1)—H(2)	109.5	O(6)—C(6)—H(17)	109.5
O(1)—C(1)—H(3)	109.5	O(6)—C(6)—H(18)	109.5
H(1)—C(1)—H(2)	109.5	H(16)—C(6)—H(17)	109.5
H(1)—C(1)—H(3)	109.5	H(16)—C(6)—H(18)	109.5
H(2)—C(1)—H(3)	109.5	H(17)—C(6)—H(18)	109.5
Cl(1)—Pd(1)—P(2)—O(4)	−151.9 (2)	O(1)—P(1)—O(2)—C(2)	170.3 (5)
Cl(1)—Pd(1)—P(2)—O(5)	90.0 (2)	O(2)—P(1)—O(1)—C(1)	73.0 (6)
Cl(1)—Pd(1)—P(2)—O(6)	−27.2 (2)	O(1)—P(1)—O(3)—C(3)	−52.8 (7)
Cl(2)—Pd(1)—P(1)—O(1)	98.3 (2)	O(3)—P(1)—O(1)—C(1)	−177.4 (6)
Cl(2)—Pd(1)—P(1)—O(2)	−18.5 (2)	O(2)—P(1)—O(3)—C(3)	52.8 (7)
Cl(2)—Pd(1)—P(1)—O(3)	−142.6 (2)	O(3)—P(1)—O(2)—C(2)	62.1 (6)
P(1)—Pd(1)—P(2)—O(4)	27.1 (2)	Pd(1)—P(2)—O(4)—C(4)	175.4 (5)
P(1)—Pd(1)—P(2)—O(5)	−91.0 (2)	Pd(1)—P(2)—O(5)—C(5)	−71.2 (6)
P(1)—Pd(1)—P(2)—O(6)	151.9 (2)	Pd(1)—P(2)—O(6)—C(6)	−58.1 (5)
P(2)—Pd(1)—P(1)—O(1)	−81.8 (2)	O(4)—P(2)—O(5)—C(5)	165.0 (6)
P(2)—Pd(1)—P(1)—O(2)	161.4 (2)	O(5)—P(2)—O(4)—C(4)	−61.6 (7)
P(2)—Pd(1)—P(1)—O(3)	37.3 (2)	O(4)—P(2)—O(6)—C(6)	70.5 (5)
Pd(1)—P(1)—O(1)—C(1)	−52.9 (6)	O(6)—P(2)—O(4)—C(4)	44.8 (7)
Pd(1)—P(1)—O(2)—C(2)	−65.9 (6)	O(5)—P(2)—O(6)—C(6)	178.7 (5)
Pd(1)—P(1)—O(3)—C(3)	−177.3 (5)	O(6)—P(2)—O(5)—C(5)	55.1 (6)

Symmetry codes: (i)  $x-1/2, -y+1/2, z-1/2$ ; (ii)  $x+1, y, z$ ; (iii)  $x-1/2, y-1/2, z$ ; (iv)  $x, -y, z+1/2$ ; (v)  $x+1/2, -y+1/2, z+1/2$ ; (vi)  $x+1/2, y+1/2, z$ ; (vii)  $x, -y, z-1/2$ ; (viii)  $x-1, y, z$ ; (ix)  $x-1/2, y+1/2, z$ ; (x)  $x-1, -y, z-1/2$ ; (xi)  $x+1/2, y-1/2, z$ ; (xii)  $x-1/2, -y+1/2, z+1/2$ ; (xiii)  $x+1/2, -y+1/2, z-1/2$ ; (xiv)  $x+1, -y, z+1/2$ .

Fig. 1

